A COMSOL Multiphysics®-based Model for Simulation of Methane-Hydrate Dissociation by Injection of Superheated CO$_2$
Experimental setup

CTD

Raman

IR

Sample

CO₂

CH₄

PTS

Bulk fluid sampling

H₂O (RT)

PTS

CO₂

CH₄

CO₂

CH₄

Sample

-7°C – + 10°C

95°C
Experiment steps

$T_1, P_1$

Sand
Water
CH$_4$-Hydrate

$T_2 > T_1, P_1$

Sand
Water
CH$_4$-Hydrate

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

CO$_2$

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

CO$_2$

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

CO$_2$

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

CO$_2$

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

CO$_2$

$T_1, P_1$

Sand
Water
CO$_2$-CH$_4$-Hydrate

CO$_2$
Experimental conditions

- 4 experiments at different p/T-conditions
  - 1) 2°C / 13 MPa
  - 2) 8°C / 13 MPa
  - 3) 10°C / 13 MPa
  - 4) 8°C / 8 MPa

- CO₂ injection
  - 95°C
  - 2-5 ml/min
Reactions of interest

Under stability conditions:
\[
\text{CH}_4\text{-Hydrate} \leftrightarrow \text{CH}_4(\text{aqueous}) + \text{H}_2\text{O} \\
\text{CO}_2(\text{aqueous}) + \text{H}_2\text{O} \leftrightarrow \text{CO}_2\text{-Hydrate} \\
\text{CO}_2(\text{aqueous}) \leftrightarrow \text{CO}_2(\text{liquid}) \\
\text{CH}_4(\text{aqueous}) \leftrightarrow \text{CH}_4(\text{gas})
\]

At dissociating conditions:
\[
\text{CH}_4\text{-Hydrate} \rightarrow \text{CH}_4(\text{gas}) + \text{H}_2\text{O} \\
\text{CO}_2\text{-Hydrate} \rightarrow \text{CO}_2(\text{liquid}) + \text{H}_2\text{O}
\]

- In CSTR model, mass and energy balance are solved explicitly and coupled to the reactivity in the system.
1. **Bulk model approach**

Using CSTR (continuous stirred tank reactor) and Batch

- Assuming the reactor as a non-isothermal CSTR
- Assuming the effects caused by transport limitations are negligible or included into the estimated effective rate parameters
- All properties (T, P, concentrations) are averaged over the reactor and therefore have one value.
CSTR modeling Pros and cons

**Pros:**
- Fast, effective and computationally cheap
- Good approximations of dynamics at small-scales
- Quick and easy for sensitivity analysis
- Better numerical convergence on higher non-linearities raised by complicated definitions of reaction rates – multiple reactions

**Cons:**
- There is one averaged value for quantities like pressure, temperature and chemical concentrations
- CSTR can not address spatial properties and thus is not precise enough for reservoir modeling
- Medium geometry, inlet and outlet positions, shape of reservoir and etc. don’t influence the outcomes.
- Transport limitation effects are neglected.
CSTR Model preliminary results

- Total CH4 in the system for experiment 1 and experiment 3.
  - 1) 2°C / 13 Mpa
  - 3) 10°C / 13 MPa

- CO2 injection
  - 95°C
  - 2-5 ml/min
CSTR Model preliminary results

- Total CO2 in the system for experiment 1 and experiment 3.

- 1) 2°C / 13 Mpa
- 3) 10°C / 13 MPa

- CO2 injection
  - 95°C
  - 2-5 ml/min
CSTR results for experiment 1

- Exp (1) 2°C / 13 Mpa
- \( \text{CO}_2 \) injection
- 95°C
- 2-5 ml/min

\( \text{CO}_2 \) stability temperature = 282.5 K
\( \text{CH}_4 \) stability temperature = 287 K
CSTR results for experiment 1

- Exp (1) 2°C / 13 Mpa
- CO₂ injection
- 95°C
- 2-5 ml/min

Hydrate amount in the system (Exp 1)
CSTR results for experiment 3

- Exp (3) 10°C / 13 MPa
- CO₂ injection
- 95°C
- 2-5 ml/min

CH₄ stability temperature = 287 K
CO₂ stability temperature = 282.5 K
CSTR results for experiment 3

- Exp (3) 10°C / 13 MPa
- CO₂ injection
- 95°C
- 2-5 ml/min

Hydrate amounts in the system (Exp 3)
2. Reservoir modeling approach
Solving the flow equations for spatial geometries

Average Temperature = 330 (K)
Two-phase fluid flow transport

• In order to include the spatial movement of the components in the model, development of a two-phase platform has been started.

• In following a non-wet phase pushes the wetting phase out of an experimental column.
Two-phase fluid flow
Medium and meshing

- At inlet non-wet phase (CO$_2$) enters the medium and wetting-phase (Water) depletes from outlet.
2-phase Model preliminary results

- Pressure in the medium over time (from top to bottom)
2-phase Model preliminary results

- Wetting phase saturations over time (from top to bottom)
2-phase Model preliminary results

- Temperature over time (from top to bottom)

![Temperature maps](image)

Steady state
Take-away messages

• Two different modeling approaches for methane-hydrate dissociation were presented.

• CSTR-based model is quick and provide a platform for 3-phase solutions which are not currently feasible in reservoir models.

• Parameter study is only feasible with 2D or CSTR models since the computational time of the 3D models is very high.

• In turn, 3D models enable us to discover some details that 2D models can’t show.

Thank you for your attention and see you at Poster #8